Introduction to the Argonne Training Program on Extreme-Scale Computing (ATPESC)

Paul Messina

Director of Science

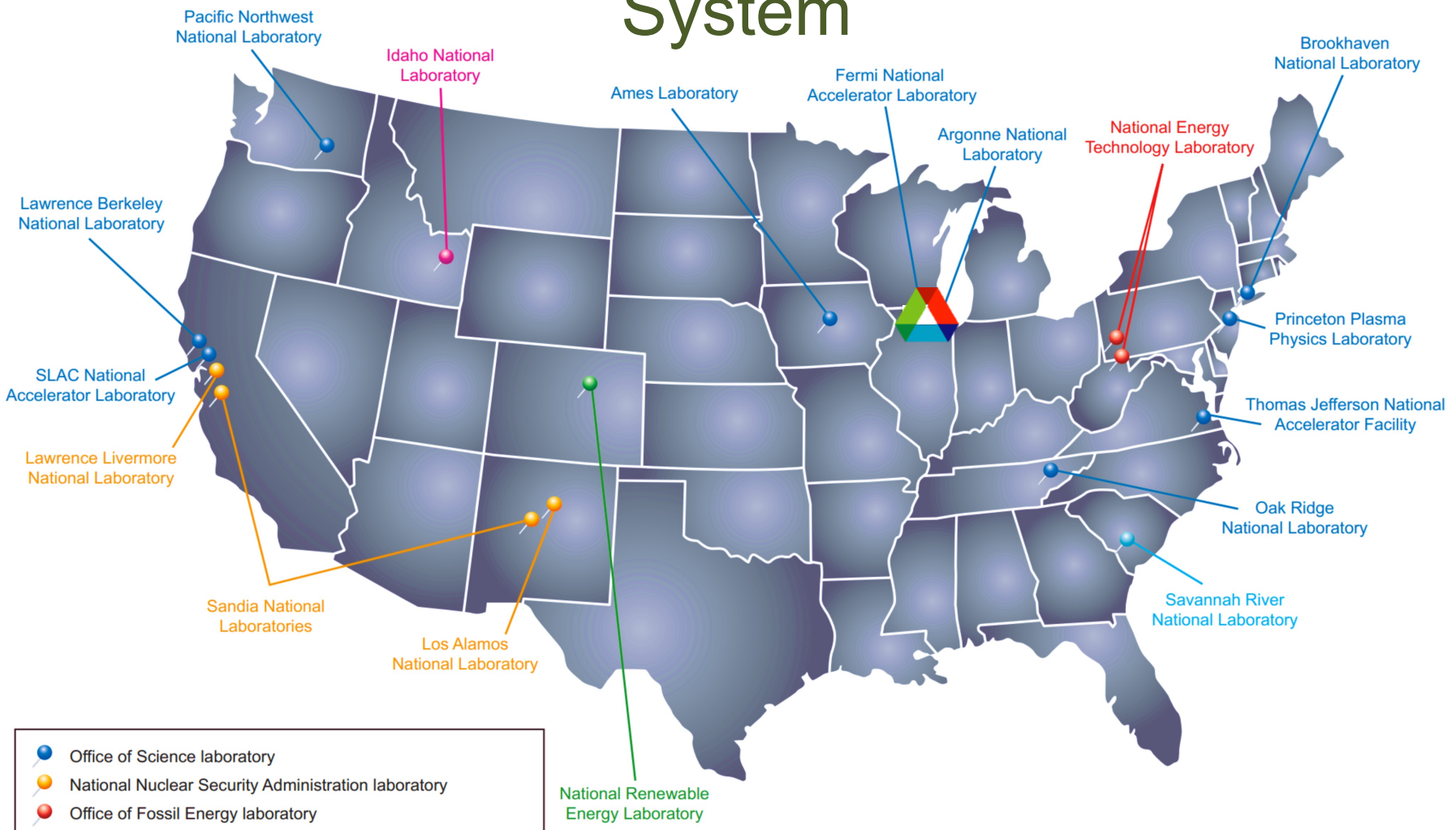
Argonne Leadership Computing Facility

Argonne National Laboratory

Outline

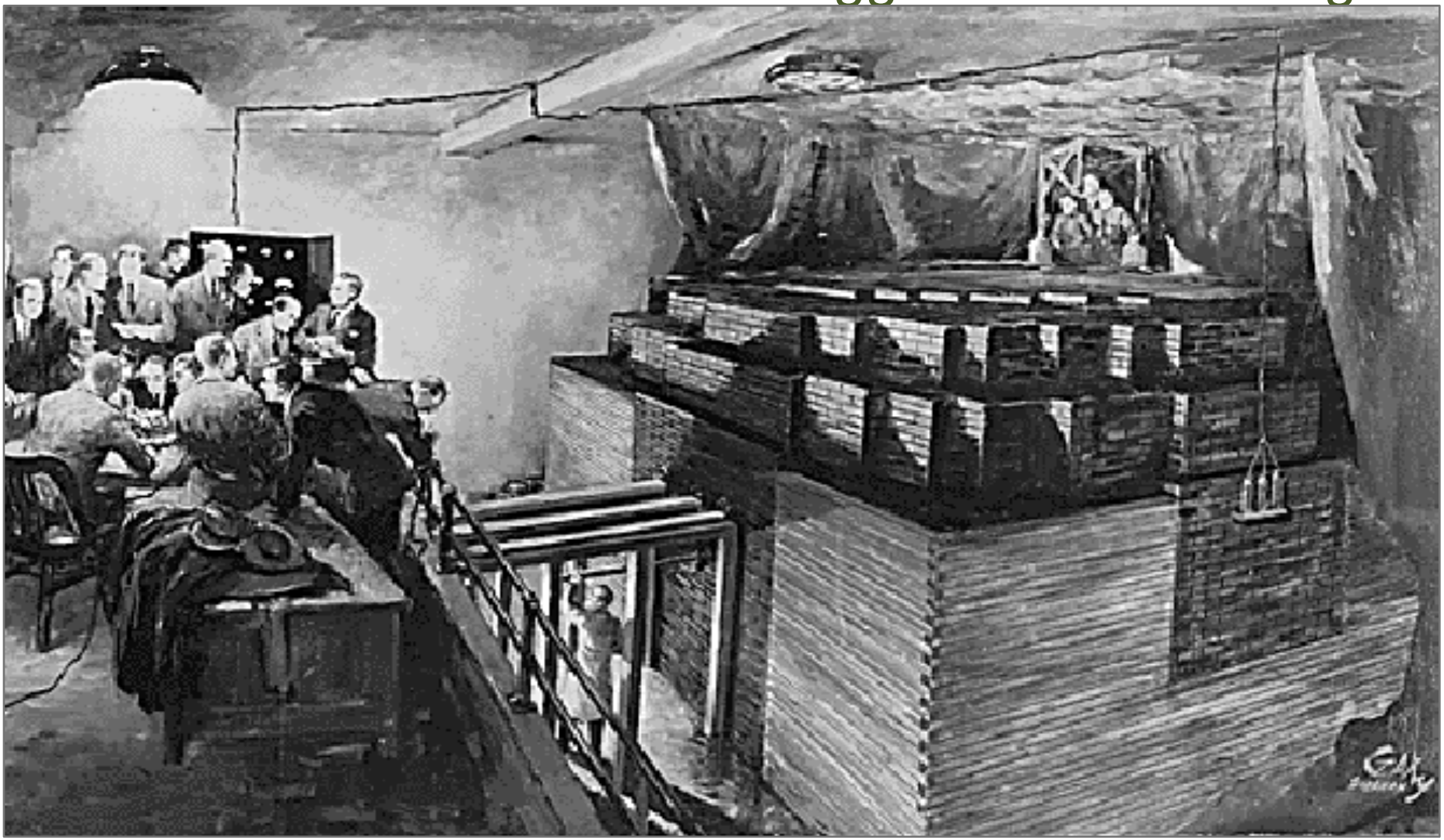
- Welcome
- A few words about Argonne National Laboratory
- Motivation of the ATPESC
- The curriculum
- Logistics and reminders

Argonne – a part of DOE National Laboratory System



U.S. DEPARTMENT OF ENERGY

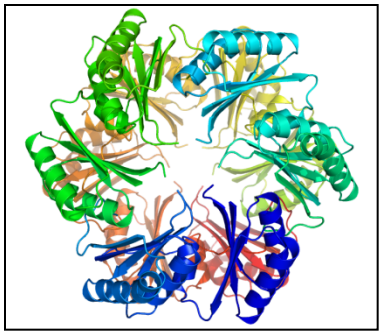
The origin of Argonne National Laboratory: CP-1 under the stands of Stagg field of U. Chicago



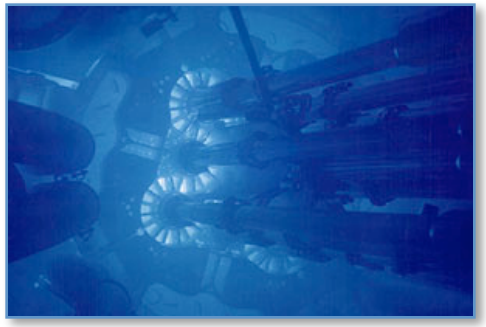
Chicago Pile-1 was the world's first artificial nuclear reactor. The first man-made self-sustaining nuclear chain reaction was initiated on December 2, 1942

Argonne's mission: To provide science-based solutions to pressing global challenges

Energy Science



Environmental Sustainability

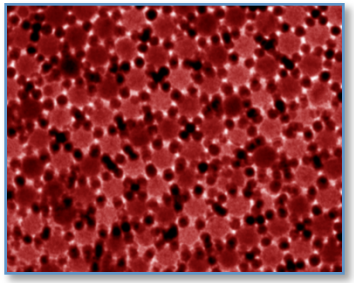


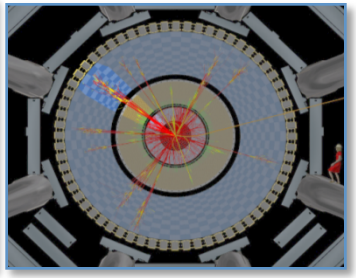
Nuclear and National Security

Use-Inspired Science and Engineering…

…Discovery and Transformational Science and Engineering

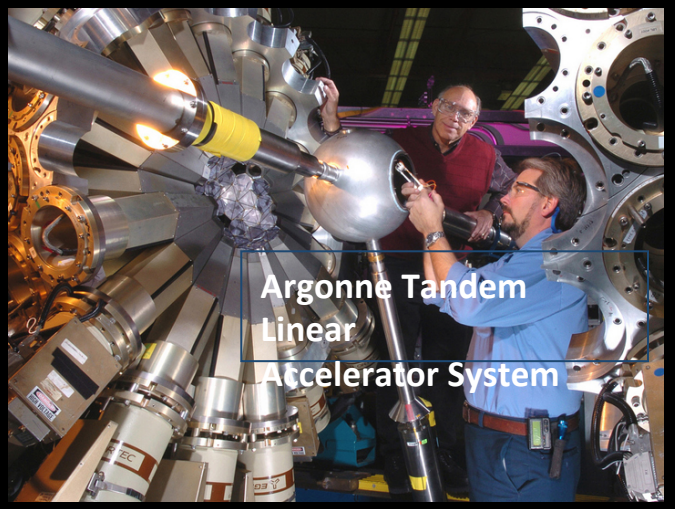
Major User Facilities

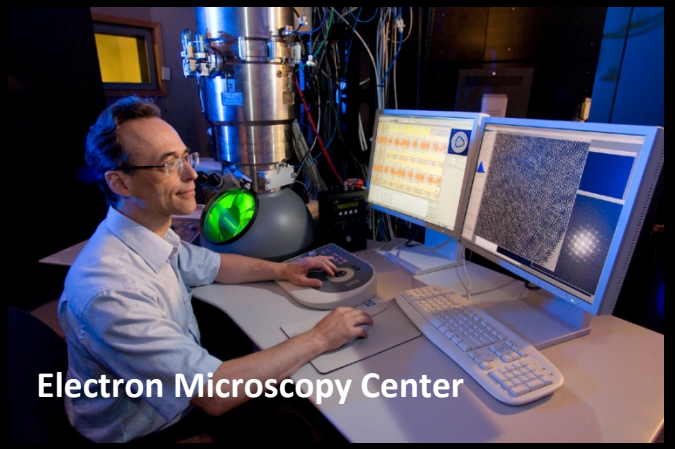




Science and Technology Programs

Major Scientific User Facilities at Argonne





AVIDAC: Argonne's Version of the Institute's Digital Arithmetic Computer: 1949-1953

"Moll" Flanders, Director
Jeffrey Chu, Chief Engineer

- **AVIDAC: based on prototype at the Institute for Advanced Study in Princeton**
- **Margaret Butler wrote AVIDAC's interpretive floating-point arithmetic system**
  - Memory access time: 15 microsec
  - Addition: 10 microsec
  - Multiplication: 1 millisec
- **AVIDAC press release: 100,000 times as fast as a trained "Computer" using a desk calculator**

Early work on computer architecture

Margaret Butler helped assemble the ORACLE computer with ORNL Engineer Rudolph Klein. In 1953, ORACLE was the world's fastest computer, multiplying 12-digit numbers in .0005 seconds (2Kop/s). Designed at Argonne, it was constructed at Oak Ridge.

Tour of Argonne National Laboratory Saturday August 8 1:00 – 6:00 p.m.

- **The Advanced Photon Source (APS)** is one of the most technologically complex machines in the world. The APS provides the brightest high-energy X-ray beams in the Western Hemisphere to more than 6,000 scientists each year from every U.S. state, the District of Columbia, Puerto Rico, and countries in the world.
- **The Nuclear Energy Exhibit (building 208)** showcases Argonne's rich heritage in the development of nuclear reactors and its current role in the development of next-generation reactors and fuel cycle technologies.
- **The Argonne Leadership Computing Facility (ALCF)** is one half of the U.S. Department of Energy's (DOE) Leadership Computing Facility, which deploys two diverse high-performance computer architectures that are 10 to 100 times more powerful than typical research computing systems
- **Buses will take us from Pheasant Run to Argonne and back**
- **Please sign up ASAP if you would like to go on the tour**
- **Deadline for signing up**

Aerial view of Argonne National Laboratory

Motivation for the ATPESC

- **Today's most powerful supercomputers have complex hardware architectures and software environments**
  - and even greater complexity is on the horizon from next-generation and exascale systems
- **The scientific and engineering applications that are tackled with these systems are themselves complex**
- **There is a critical need for specialized, in-depth training for the computational scientists poised to facilitate breakthrough science and engineering using these systems**

The DOE Leadership Computing Facility

- Collaborative, multi-lab, DOE/SC initiative ranked top national priority in ***Facilities for the Future of Science: A Twenty-Year Outlook.***
- Mission: Provide the computational and data science resources required to solve the most important scientific & engineering problems in the world.
- Highly competitive user allocation program (INCITE, ALCC).
- Projects receive 100x more hours than at other generally available centers.
- LCF centers partner with users to enable science & engineering breakthroughs (Liaisons, Catalysts).

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

Leadership Computing Facility systems

	Argonne LCF	Oak Ridge LCF
System	IBM Blue Gene/Q	Cray XK7
Name	Mira	Titan
Compute nodes	49,152	18,688
Node architecture	PowerPC, 16 cores	AMD Opteron, 16 cores NVIDIA K20x (Kepler) GPU
Processing Units	786,432 Cores	299,008 x86 Cores + 18,688 GPUs
Memory per node, (gigabytes)	16	32 + 6
Peak performance, (petaflops)	10	27

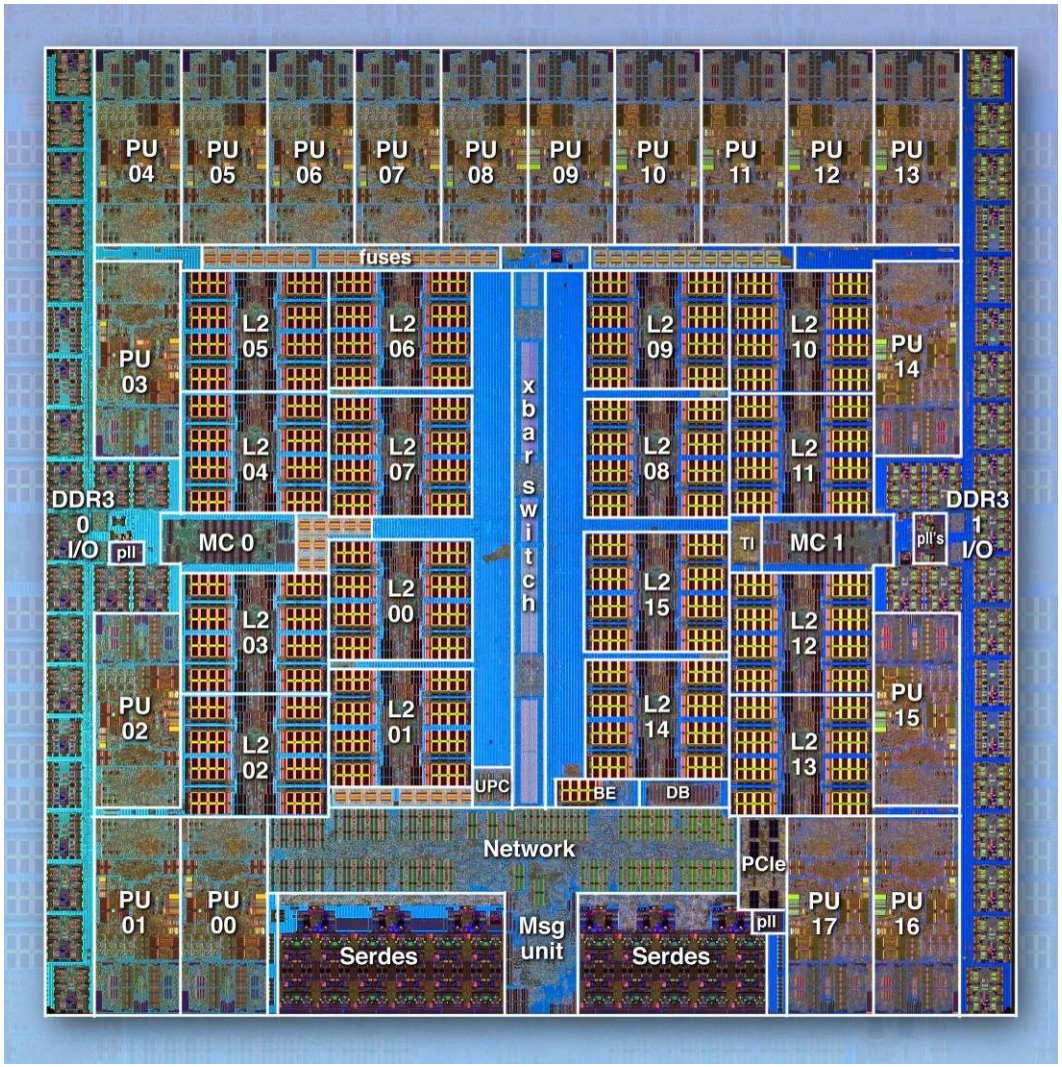
ALCF Systems

- ***Mira* – BG/Q**
  - 49,152 nodes / 786,432 cores
  - 786 TB of memory
  - Peak flop rate: 10 PetaFLOPs
  - 3,145,728 hardware threads
- ***Vesta (T&D)* - BG/Q**
  - 2,048 nodes / 32,768 cores
- ***Cetus (debug)* - BG/Q**
  - 4,096 nodes / 65,5368 cores

- ***Cooley (visualization & data analysis)* – Cray CS**
  - 126 nodes, each with
    - Two Intel Xeon E5-2620 Haswell 2.4 GHz 6-core processors
    - NVIDIA Tesla K80 graphics processing unit with 24 GB memory
    - 384 GB DDR4 memory
- **Storage**
  - Scratch: 28.8 PB raw capacity, 240 GB/s bw (GPFS)
  - Home: 1.8 PB raw capacity, 45 GB/s bw (GPFS)

BlueGene/Q Compute Chip

System-on-a-Chip design : integrates processors, memory and networking logic into a single chip



- **360 mm² Cu-45 technology (SOI)**
  - ~ 1.47 B transistors
- **16 user + 1 service processors**
  - plus 1 redundant processor
  - all processors are symmetric
  - L1 I/D cache = 16kB/16kB
  - L1 prefetch engines
- **Crossbar switch**
  - Connects cores via L1P to L2 slices
- **Central shared L2 cache**
  - 32 MB eDRAM
  - 16 slices
- **Dual memory controller**
  - 16 GB external DDR3 memory
  - 42.6 GB/s
- **Chip-to-chip networking**
  - Router logic integrated into BQC chip
  - DMA, remote put/get, collective operations
  - 11 network ports
- **External IO**
  - PCIe Gen2 interface

DOE ASCR Computing Upgrades At a Glance

System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
Name Planned Installation	**Edison**	**TITAN**	**MIRA**	**Cori 2016**	**Summit 2017-2018**	**Theta 2016**	**Aurora 2018-2019**
System peak (PF)	2.6	27	10	> 30	150	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM) +1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR-IB	Aries	2nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/ s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

Aurora

- **Homogeneous**
- **Many-core**
  - Four hardware threads/core
- **Self-hosted**
- **Water cooled**

- **18x *Mira* speed**
- **2.7x *Mira* peak power consumption**
- **Similar node count to *Mira***
- **Intel Architecture (x86-64) Compatibility**

Theta

- **Homogeneous**
- **Many-core**
  - Four hardware threads/core
- **Self-hosted**
- **Water cooled**

- **0.85x *Mira* speed**
- **0.35x *Mira* peak power consumption**
- **>2500 nodes**
- **Intel Architecture (x86-64) Compatibility**

Curriculum tracks/sessions and their leaders

- Architectures – Pete Beckman
- Programming models and languages – Rusty Lusk and Rajeev Thakur
- Numerical algorithms and software -- Lois McInnes and Lori Diachin
- Community codes and software engineering – Katherine Riley and Anshu Dubey
- Toolkits and frameworks – Kalyan Kumaran and Scott Parker
- Visualization and data analysis – Mike Papka and Joe Insley
- Data-intensive computing and I/O – Rob Ross and Rob Latham

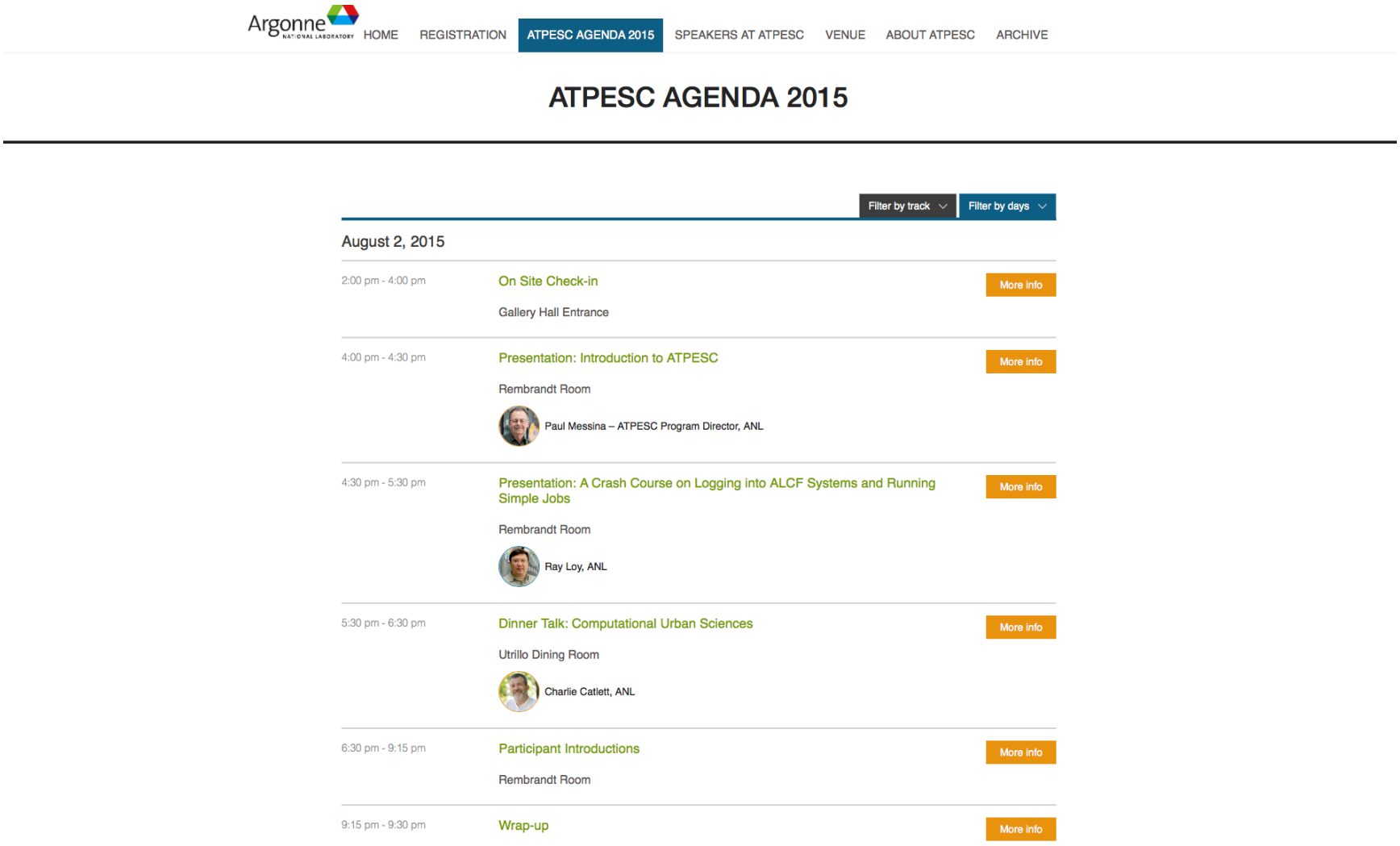
Dinner talks

- **Purpose: present additional topics that will probably be relevant to your research at some point in your career – but in any case interesting**
- **Nine dinner talks**

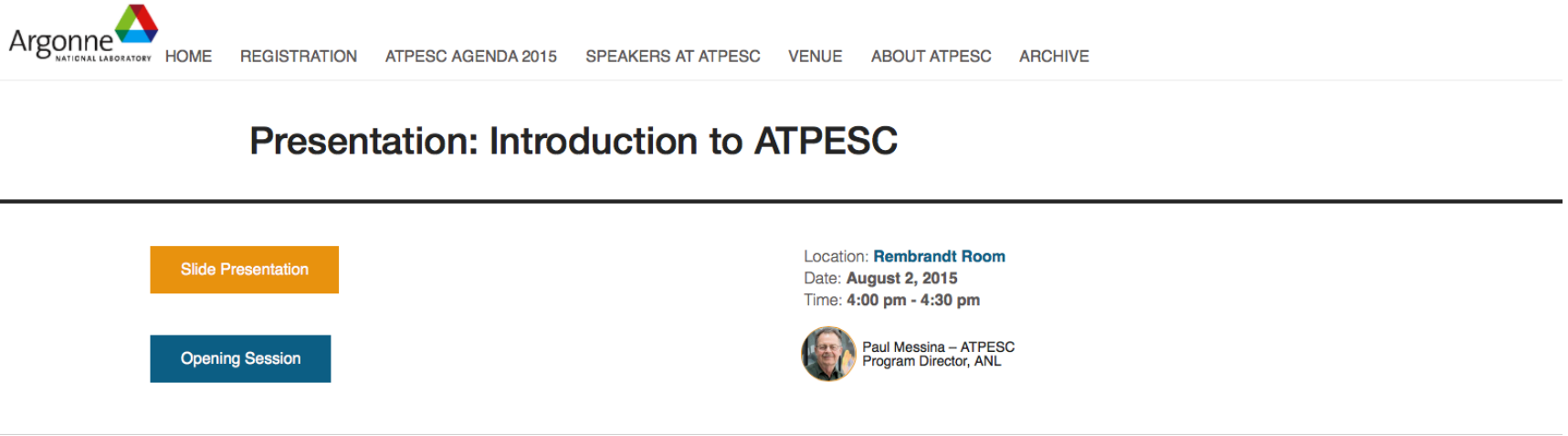
Yes, the ATPESC is an intense program

- **Many lectures every day, followed by evening hands-on sessions**
- **Ideally we would cover all topics in more depth but the result would be a six-week program**
  - But few people's schedules would allow them to participate
- **Note the 8:30 a.m. starting time, dinner at 5:30 p.m. right after the end of the afternoon lectures, evening sessions**
- **Slides will be posted online as soon as available**
  - **Show how to find the slides on the agenda**

Go to the ATPESC Agenda, click on More Info



Then click on Slide Presentation



Thank you, DOE Office of Advanced Scientific Computing Research (ASCR)

- **This training program was made possible by funding from the Research Division of the Advanced Scientific Computing Research program of the Department of Energy's (DOE) Office of Science**
- **The initial funding was for three years (2013-2015)**
  - We have requested funding for 2016-2018
- **Help us improve the training program**
  - Track evaluations
  - Overall program evaluation
  - Conversations or emails to any of us

Surveys

- **Help us improve the training program**
  - Track evaluations
  - Overall program evaluation
  - Conversations or emails to any of us
- **Please fill out the online evaluation surveys on each track and the overall program**
  - at the end of each track, you will receive an email from Chel@alcf.anl.gov with a link to that track's evaluation
  - Respond by the morning of the next day to be eligible for the prize raffle
  - Chel Lancaster is coordinating the evaluations and will be available to answer questions or help

Suggestions from previous year's surveys adopted this year

- Tour of Argonne
- Pre-event exercises
- More hands-on exercises during lectures
- Participant introductions

Participant introductions

- **One minute (60 seconds) to say something about yourself so that participants will know who has common interests**
- **Right after dinner we will go to the main lecture room upstairs (Rembrandt)**
- **Get drink at the bar that is in the hallway outside the room and sit where you like**
  - Each of you has a drink ticket in your badge holder
  - Additional drinks are on a cash basis

Paul Messina

- **Position: Ph.D. student, applied mathematics, University of Cincinnati**
- **Research background:**
  - Solution of elliptic PDEs with singularities
  - Mathematical software
- **Research interests:**
  - Parallel computer architectures
- **Personal interests**
  - Sailing
- **Personal background:**
  - Had lived in four countries by the time I was 14 years old

Participant introduction logistics

- If you have a slide about yourself for the participant introduction and you have not yet sent it, please email it to vdoyle@anl.gov or support@extremecomputingtraining.anl.gov
- Or, while people are getting drinks, please bring it on a USB stick or come to the podium with your laptop and I will have a USB stick
- I will arrange the slides in alphabetic order and call you to the podium to present it
- For those of you without slides I will ask you to come forward, in alphabetic order

Slack chat system

- You have all received an invitation to join the #atpesc2015 channel
- We set it up so that you can engage in one-on-one private communications with each other, and with us.

ATPESC Social Media

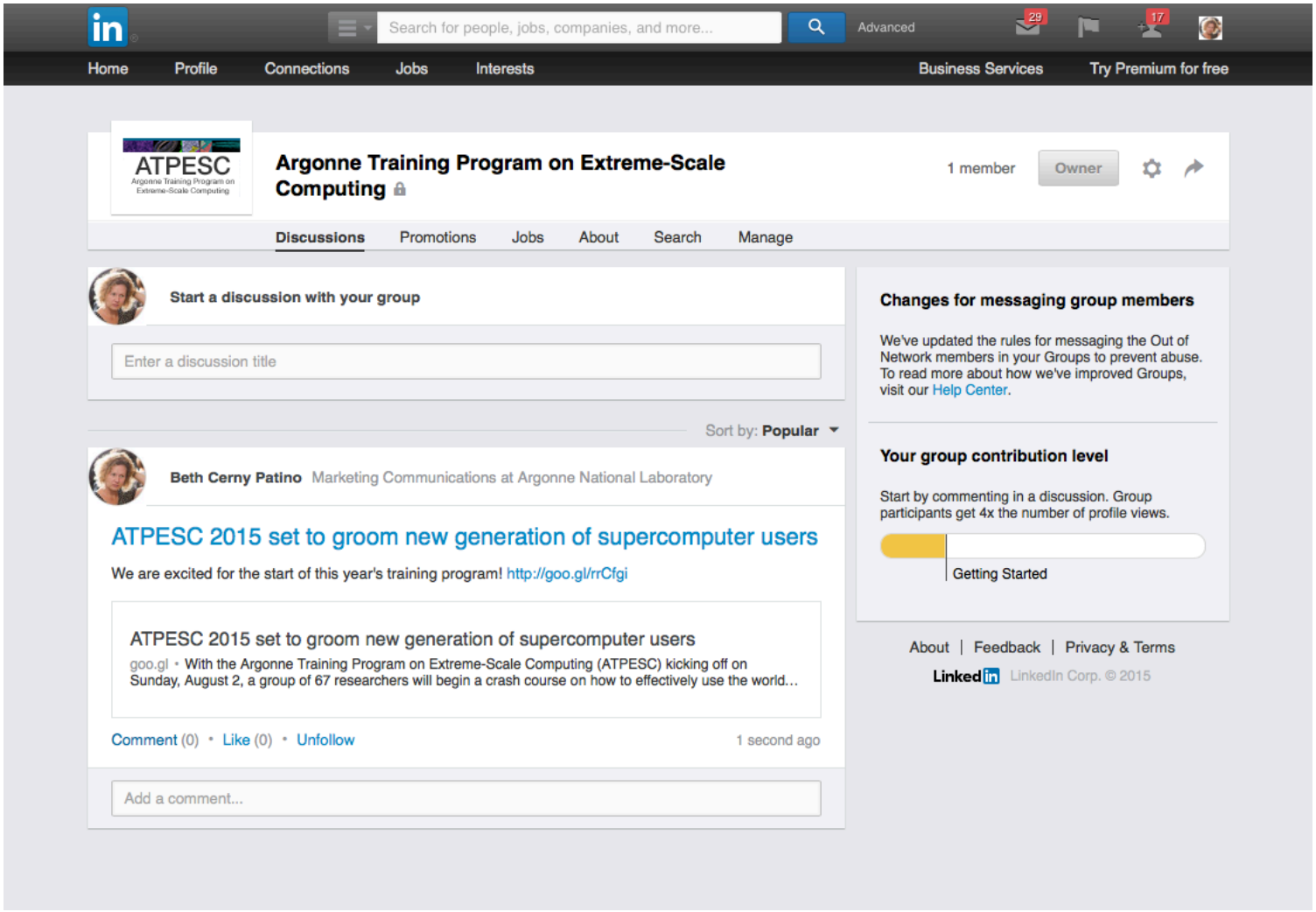
ATPESC Social Media

Like Us on Facebook

- **Share your experience on the ATPESC Facebook page**
  - Share your photos
  - Share something that you didn't know before
  - Share how this will help your career
  - Share how wonderful the lecturers are
  - Share interesting articles on Computational Science using HPC
  - **facebook.com/atpesc**

    - The page is open to the public and allows anyone to add postings, photos, and videos. All posts will be moderated by ALCF staff.

ATPESC Social Media



ATPESC Social Media

Join our ATPESC LinkedIn Group

- **Open to all ATPESC alumni; private for members-only**
  - Start a discussion
  - Share job openings
  - Share interesting articles related to the group
  - Share the value of your ATPESC experience
  - Share opportunities
  - Search group name: **Argonne Training Program on Extreme-Scale Computing**
  - URL: **linkedin.com/grp/home?gid=8355790**

  - The ATPESC group on LinkedIn is closed and only members can see and participate in group discussions.

General Logistics

- **All lectures and hands-on sessions in Rembrandt room**
- **All meals in Utrillo room on ground floor**
  - Lunch and dinner presentations will be in this room
- **Other rooms in ground floor may be used as needed**
- **Wi-fi SSID in this building is Argonne2015**
- **Password is alabs2015**

Diagram of Meeting Rooms: Second Floor

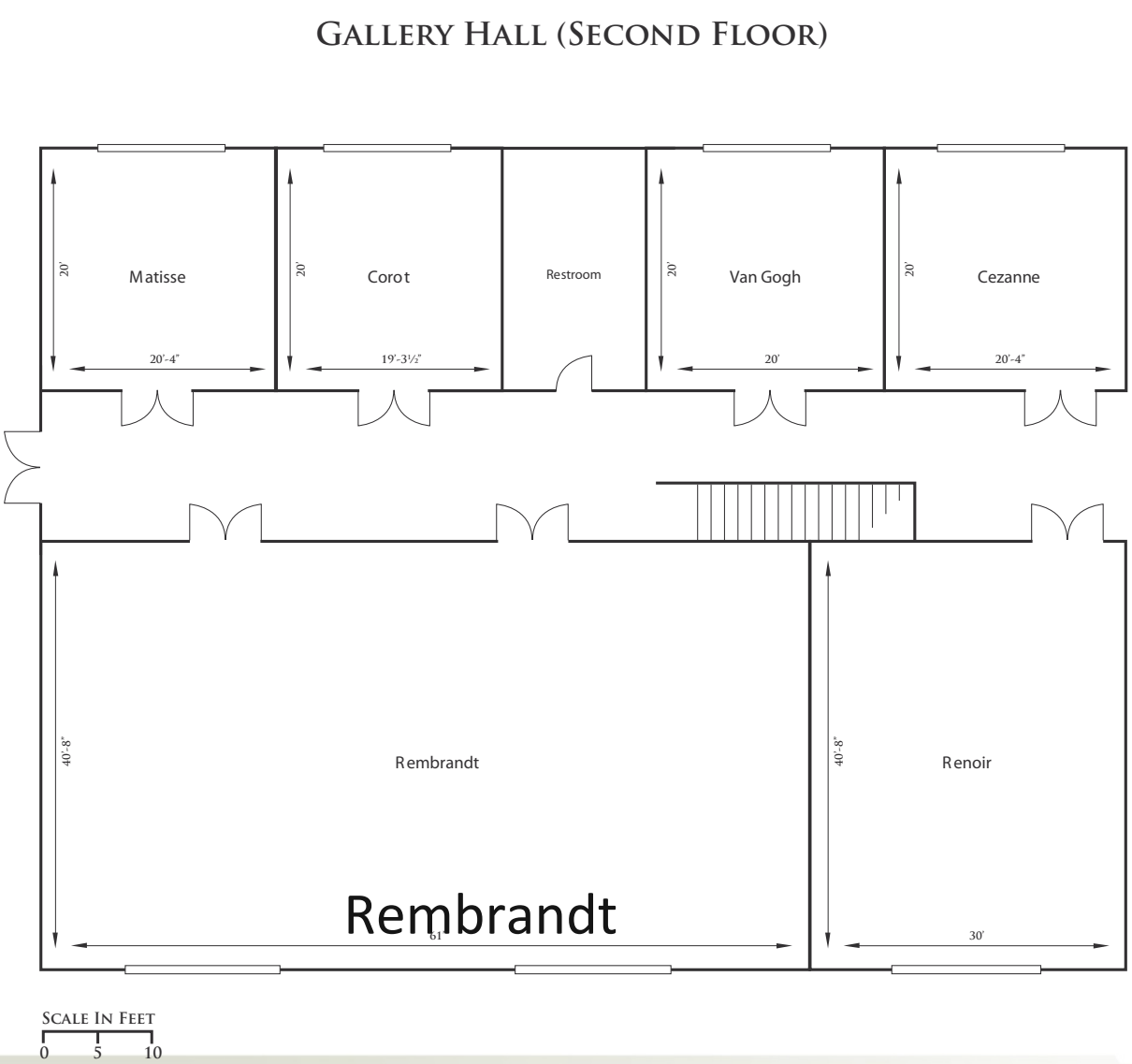
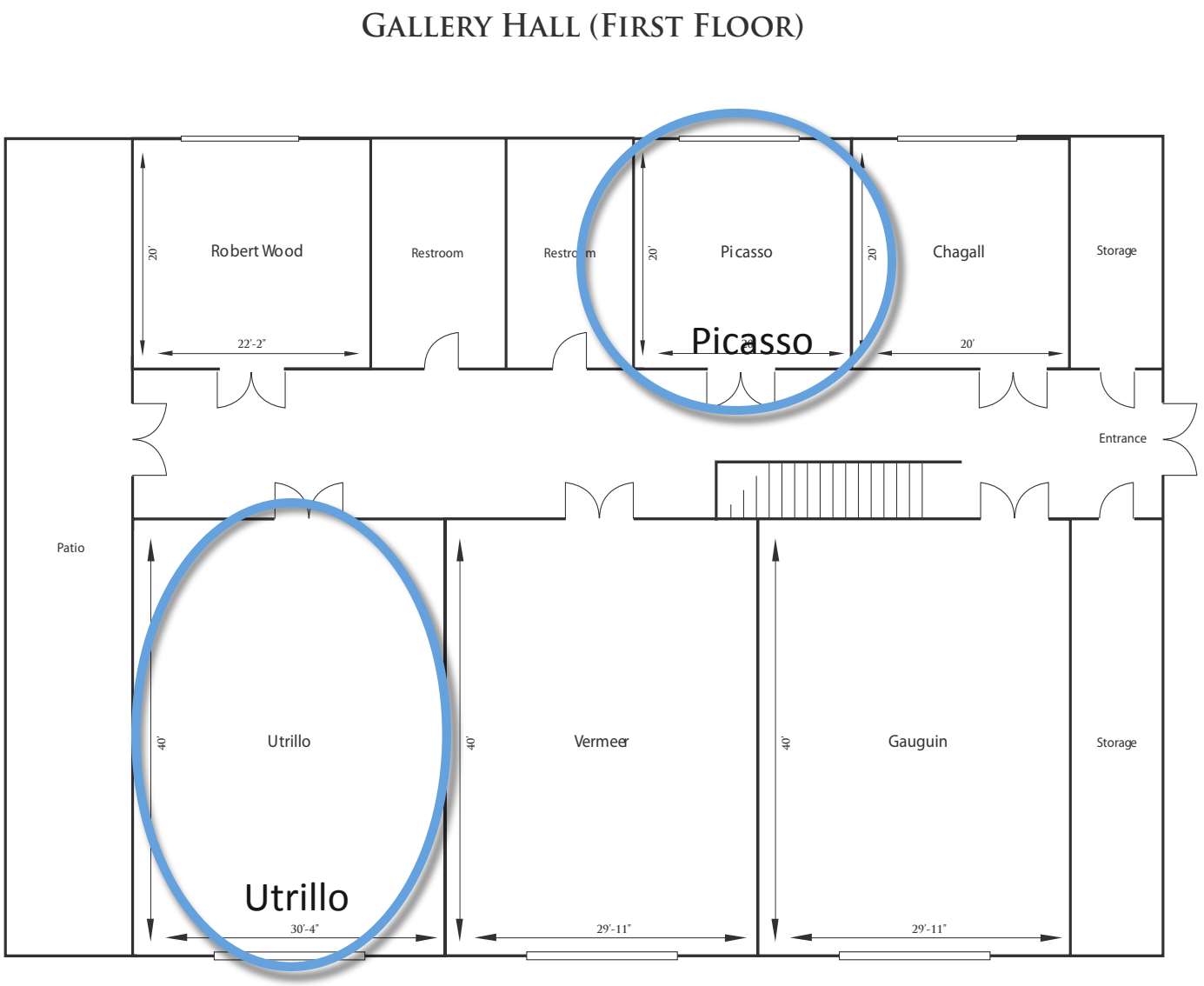


Diagram of meeting rooms: Ground floor



Whom to ask for help

- Local arrangements
  - Cheryl Zidel
  - Ashley Boyle
  - Ginny Doyle
  - Julie Smagacz
  - (one of them will be in the Picasso room almost always)
- Surveys
  - Chel Lancaster
- Computing issues
  - Ray Loy
  - Robert Scott
  - Adam Scovel
  - Others TBD

After the ATPESC

Some opportunities

Allocation Programs at the LCFs

	60% INCITE		30% ALCC		10% Director's Discretionary	
Mission	High-risk, high-payoff science that requires LCF-scale resources*		High-risk, high-payoff science aligned with DOE mission		Strategic LCF goals	
Call	1x/year – (Closes June)		1x/year – (Closes February)		Rolling	
Duration	1-3 years, yearly renewal		1 year		3m,6m,1 year	
Typical Size	30 - 40 projects	50M - 500M core-hours/yr.	5 - 10 projects	10M – 300+M core-hours/yr.	100s of projects	.5M – 10M core-hours
Review Process	Scientific Peer-Review	Computational Readiness	Scientific Peer-Review	Computational Readiness	Strategic impact and feasibility	
Managed By	INCITE management committee (ALCF & OLCF)		DOE Office of Science		LCF management	
Readiness	**High**		**Medium to High**		**Low to High**	
Availability	Open to all scientific researchers and organizations ***Capability > 131,072 cores (16.7% of Mira)***					

Educational and Job Opportunities @ ALCF

- **Research Efforts**
  - Computational Science
  - Computer Science
  - Technical Communication
- **Margaret Butler Fellowship in Computational Science**
- **ALCF Director's postdoctoral program**
- **Divisional postdoctoral positions**
- **PhD dissertation support**
- **Undergraduate and graduate internships**
  - And advanced high-school level
- **Jobs at the ALCF**
  - https://www.alcf.anl.gov/about/careers

For information on the educational and postdoctoral programs at Argonne National Laboratory

- http://www.dep.anl.gov

Summary

- Thanks in advance to all of you for taking two weeks of your summer to participate in this program
- Questions?

Next: Crash course: Running MPI Programs on the ALCF Blue Gene/Q